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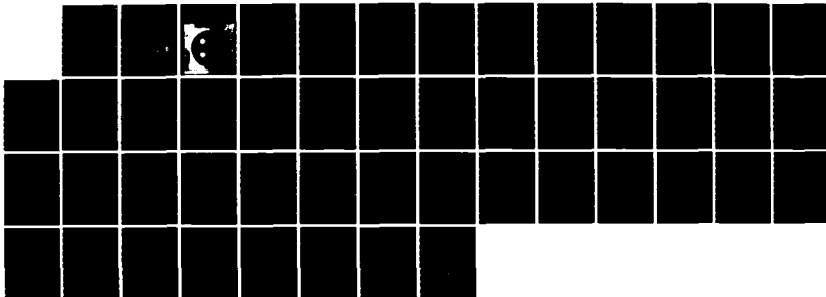
NUMERICAL SCHEMES FOR THE ESTIMATION OF FUNCTIONAL  
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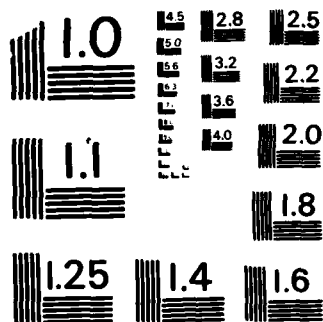
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REPORT DOCUMENTATION PAGE		READ INSTRUCTIONS BEFORE COMPLETING FORM
1. REPORT NUMBER <b>AFOSR-TR- 86-0260</b>	2. GOVT ACCESSION NO.	3. RECIPIENT'S CATALOG NUMBER
4. TITLE (and Subtitle) Numerical Schemes for the Estimation of Functional Parameters in Distributed Models for Mixing Mechanisms in Lake and Sea Sediment Cores		5. TYPE OF REPORT & PERIOD COVERED <i>Interim</i>
6. AUTHOR(s) H.T. Banks and I.G. Rosen		6. PERFORMING ORG. REPORT NUMBER
7. PERFORMING ORGANIZATION NAME AND ADDRESS Lefschetz Center for Dynamical Systems Division of Applied Mathematics Brown University, Providence, RI 02912		8. CONTRACT OR GRANT NUMBER(s) <i>0398</i> AFOSR-84- <del>0398</del>
9. CONTROLLING OFFICE NAME AND ADDRESS AFOSR/NM (Dr. Marc Jacobs) Bolling Air Force Base Washington, DC 20332		10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS <i>6.1102F, 2304, A1</i>
11. MONITORING AGENCY NAME & ADDRESS (if different from Controlling Office)		12. REPORT DATE October 1985
		13. NUMBER OF PAGES 43
		14. SECURITY CLASS. (of this report) unclassified
		15a. DECLASSIFICATION/DOWNGRADING SCHEDULE
16. DISTRIBUTION STATEMENT (of this Report)  Approved for public release: distribution unlimited		
17. DISTRIBUTION STATEMENT (of the abstract entered in Block 20, if different from Report)		
18. SUPPLEMENTARY NOTES		
19. KEY WORDS (Continue on reverse side if necessary and identify by block number)		
20. ABSTRACT (Continue on reverse side if necessary and identify by block number) —We consider distributed parameter models for vertical mixing in lake and sea sediment cores. Finite dimensional approximation schemes are developed for the solution of associated inverse problems. The schemes permit one to estimate temporally and spatially varying functional parameters which appear		

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Numerical Schemes for the Estimation of Functional Parameters in  
Distributed Models for Mixing Mechanisms in Lake and Sea Sediment Cores.<sup>†</sup>

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ABSTRACT

We consider distributed parameter models for vertical mixing in lake and sea sediment cores. Finite dimensional approximation schemes are developed for the solution of associated inverse problems. The schemes permit one to estimate temporally and spatially varying functional parameters which appear in the parabolic partial differential equations and boundary conditions constituting the models. Theoretical convergence results are established. Numerical findings are presented which demonstrate the potential of the methods. An example involving the identification of a depth dependent mixing parameter based upon volcanic ash data from the North Atlantic is included.

(\*) This research was supported in part by the National Science Foundation under NSF Grant MCS-8205355, the Air Force Office of Scientific Research under contract No. AFOSR-84-0398 and the Army Research Office under contract No. ARO-DAAG-29-83-K-0029.

(\*\*) This research was supported in part by the Air Force Office of Scientific Research under contract No. AFOSR-84-0398.

(†) Part of the research was carried out while the authors were visiting scientists at the Institute for Computer Applications in Science and Engineering (ICASE) NASA Langley Research Center, Hampton, VA, 23665 which is operated under NASA contract No. NAS1-17070.

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## 1. INTRODUCTION

In this paper we develop numerical approximation methods for the solution of inverse problems arising in the modeling of mixing mechanisms evidenced in lake and sea sediment core samples. In particular we develop methods for the estimation of temporally and spatially varying parameters in models involving distributed (partial differential equation) systems. Our work has been motivated primarily by the recent interest in models involving depth dependent mixing rates and time dependent sedimentation rates. These ideas will be discussed in detail in the next section.

The approach to be described below represents a significant improvement over an earlier treatment of the problem by the present authors (see [6]). Indeed, based upon a weak or variational formulation of the partial differential equation and boundary conditions which compose the model that is the focus of our study (as opposed to using a semigroup theoretic approach), the theory developed here leads to schemes which permit the estimation of both temporarily and spatially varying parameters under rather mild assumptions on the set of admissible parameters. No prior assumptions need be made about the "shape" of the functional parameters being estimated.

Another feature of the estimation problems that are of interest to us here which must be considered when approximation schemes are being developed is that they generally involve observations at the boundary. This poses a significant mathematical problem since many mixing models involve parabolic systems which are often formulated in the state space  $H^0$  where point evaluation is undefined. Under rather mild regularity assumptions we are able to argue that our state approximations converge in the stronger  $H^1$  and, via the Sobolev embedding theorem,  $C$  topologies. Consequently, our schemes are applicable to inverse problems in which the fit to data criterion involves

point or discrete as well as distributed observations in the spatial variable.

The general approach we take here has been used extensively to develop approximation methods for the solution of inverse problems involving distributed systems arising in a wide variety of application areas (e.g. population dispersal, physiology, large flexible spacecraft, seismic analysis, diffusion through porous media, etc.). A brief description of some of the problems and the associated approximation schemes together with a survey of the literature and a more comprehensive bibliography can be found in [1].

We provide a brief outline of the remainder of the paper. In Section 2 the sediment core mixing problem is described and previous modeling efforts are discussed. A particular model involving a diffusion/advection equation is developed in detail and associated inverse problems are posed. The identification problem is formally stated and the weak formulation of the partial differential equation together with existence, uniqueness and regularity results for solutions are discussed in Section 3. In Section 4 we describe the approximation schemes and establish convergence results. Examples and our numerical findings are given in Section 5. Our primary objective in this paper is to present our theoretical results. The numerical results discussed in Section 5 are preliminary. A more complete numerical study will be described elsewhere.

The notation we employ is standard throughout. We denote by  $H^k(a,b)$  the usual Sobolev spaces of real valued functions  $\phi$  defined on the interval  $(a,b)$  whose  $(k-1)$ st derivative,  $D^{k-1}\phi$ , is absolutely continuous and whose  $k^{th}$  derivative,  $D^k\phi$  is in  $L_2(a,b) = H^0(a,b)$ . The standard Sobolev inner products and norms are denoted by  $\langle \cdot, \cdot \rangle_k$  and  $|\cdot|_k$  respectively. For  $H^k = H^k(a,b)$  a function  $v : (t_0, t_1) \rightarrow H^k$  is said to be an element in  $H^0(t_0, t_1; H^k)$  if



$$\|v\|_{0,k} = \left\{ \int_{t_0}^{t_1} |v(t)|_k^2 dt \right\}^{\frac{1}{2}} < \infty.$$

We shall say  $v \in H^j(t_0, t_1; H^k)$  if  $v$  possesses  $j$  strong derivatives with  $v^{(i)} \in L_2(t_0, t_1; H^k)$ ,  $0 \leq i \leq j$ . Defining

$$\|v\|_{j,k} = \left\{ \sum_{i=0}^j \int_{t_0}^{t_1} |v^{(i)}(t)|_k^2 dt \right\}^{1/2}$$

for  $v \in H^j(t_0, t_1; H^k)$  we have that the spaces  $\{H^j(t_0, t_1; H^k), \|\cdot\|_{j,k}\}$  are complete. For  $j=k$ , we abbreviate notation for the norm by writing

$$\|\cdot\|_k = \|\cdot\|_{k,k}.$$

Finally for  $V$  a Hilbert space which is densely and compactly embedded in  $H^k$  and  $v \in H^0(t_0, t_1; V)$  we denote the weak derivative of  $v$ , an element in  $H^0(t_0, t_1; V')$ , by  $\dot{v}$  where  $V'$  is the dual space of  $V$ . For  $\phi \in V$  we have

$$(\dot{v}(t))(\phi) = \langle \phi, \dot{v}(t) \rangle_k$$

where the inner product in the above expression is understood to be the extension of the  $H^k$  inner product to all of  $V'$ .

## 2. Inverse Problems in Lake and Sea Sediment Analysis

Sediment formation in lakes and deep seas is of great importance to geophysical scientists who use core samples of sediment in their investigations of the history (e.g. palaeoclimatic changes) of the earth. Unfortunately, the stratigraphic records contained in these core samples have been subjected to perturbations since ocean and lake floors are in general not quiescent. Two general types of redistribution of sediment are often significant: (i) gross lateral transport via ocean and lake bottom currents, for example, through a continuous winnowing of bottom currents or through episodic currents such as turbidity currents; (ii) the mixing activities of benthic organisms near (on the order of 2-40 cm.) the sediment-water interface. This biological mixing of sediments by organisms (which leads to an interesting class of inverse problems in the analysis of sediments) is called bioturbation [24], [7] and takes place in sediment layers in bodies of water (lakes, estuaries, the deep oceans) in which bottom water is not substantially depleted of oxygen. Bioturbation is effected by different kinds of organisms such as clams, worms, crustacea, echinoderms, etc., and the mixing activities consist primarily of burrowing (e.g., for safety) and ingestion - excretion reworking of the sediment for its edible organic matter. Through the use of tracers from dated events (e.g., plutonium from atmospheric fallout from nuclear explosions, and microtektites - tiny drops of sculptured glass resulting from cosmic events), it can be determined that the biological mixing of abyssal sediments is quantitatively significant and takes place on a relatively short (in regard to geologic records) time scale (10-20 years). Furthermore, there seems to be little correlation between bioturbation mixing rates (which are highly variable) and sediment type or sediment accumulation rates. However, the degree of bioturbation and the

depth of the region in which it occurs are related to the types of organisms inhabiting a particular area.

Since bioturbation plays such a fundamental role in the alteration of geologic records, it is not surprising that geochemists, geologists, and geophysicists have in recent years attempted to understand the effects of bioturbation well enough so as to enable one to properly interpret the information contained in core samples, thereby sharpening the details in these geologic records. A number of increasingly sophisticated mathematical models along with related "inverse problems" can be found in the literature [11] [12] [13] [15] [16] [17] [18] [19]. These models typically involve some type of region or chamber (ranging from a simple well-mixed chamber to one in which mixing rates are depth dependent) in which mixing and advection or convective flow interact to vertically redistribute sediment particulate matter, volcanic ash, microtektites, radioactive tracers or other substances from episodic and nonepisodic events.

One model which, along with its variations, has enjoyed rather widespread usage involves the assumption that one has a vertically moving chamber (assumed uniform in horizontal directions) in which mixing and advective flow of material takes place and is described by one-dimensional (depth) transport equations. Depth in the chamber is represented by coordinates  $x$ ,  $0 \leq x \leq l$  and the chamber (and hence coordinate system) is assumed to be moving upward with a velocity  $V = V(t)$  (corresponding to sedimentation rate or, equivalently in this case, sediment layer buildup) so that it is always located in the top  $l$  cm. of the sediment as depicted in the figure below. Thus  $x = 0$  is always at the water-sediment

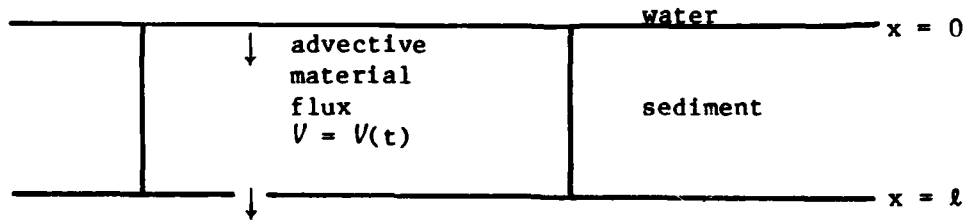


Figure 2.1

interface and the bottom of the chamber at  $x = l$  is located at that depth beyond which (it is assumed) no further changes (i.e., no bioturbation) in the historical records occur. The resulting configuration with upward velocity of the chamber can be equivalently modeled by the assumption of a fixed coordinate system for the chamber with an advective/convective flow of material downward through the chamber with velocity  $V$ . Use of the model by numerous investigators (e.g. see [18], [19]) strongly suggests that permitting a time-varying sedimentation rate in such models is important.

If  $u = u(t, x)$  is the concentration of material (e.g., shards of ash, radioactive tracer, etc.) with whose movement one is concerned and  $j = j(t, x)$  is the material flux at time  $t$  and position  $x$  in the chamber, material conservation is represented by the classical mass balance or continuity equation

$$(2.1) \quad \frac{\partial u}{\partial t} + \frac{\partial j}{\partial x} + \lambda u = 0,$$

where  $\lambda$  is a decay constant for the material ( $\lambda = 0$  if one is dealing with a conservative tracer such as microtektites). Of course, the important aspect

of any such model is the assumption one makes regarding the material flux  $j$ , which here we assume consists of a mixing component and an advective component. In this case one is justified in assuming that the bioturbation (burrowing, ingestion, etc.) takes place over a very short time scale (essentially instantaneous) in the chamber and hence perhaps can be represented by a diffusive-like flux component. The advective flux is given by  $V(t)u$  and if one assumes a Fickian flux for the bioturbation with depth dependent "bioturbation" coefficient  $D = D(x)$ , one obtains

$$(2.2) \quad j = -D \frac{\partial u}{\partial x} + Vu .$$

The assumption that  $D$  is a function of depth is motivated by ones expectation that the rate of mixing is generally higher near the well-oxygenated, densely populated surface of the sediment mixing layer; this expectation appears to be corroborated by experimental findings [11], [12], [13], [19]. A more fundamental question as to whether the biological reworking of sediment is mechanistically analogous to molecular diffusion (and hence is consistent with the Fickian flux assumption) is not so readily answered. A strict analogy would necessitate the existence of an abundance of organisms, randomly placed in the chamber, mixing the materials in a manner so as to produce a material flux proportional to concentration gradients. While this is not a very likely description of the mechanisms of biogenic mixing, one might still have a plausible quantitative analogy with diffusion if the mixing rate is rapid and sediment samples which involve a large number of independent transport events of variable duration are chosen.

For boundary conditions at the upper boundary ( $x = 0$ ) of the chamber one has the flux condition  $j(t,0) = G(t)$  when  $G$  is a possibly unknown input, while

the total flux at the lower boundary  $x = \ell$  is via advective loss through the bottom of the mixing zone and thus  $j(t, \ell) = V(t)u(t, \ell)$ . Using the constitutive relationship for  $j$  from (2.2) in these boundary conditions and in the equation (2.1), one obtains the model

$$(2.3) \quad \frac{\partial u}{\partial t} = \frac{\partial}{\partial x} \left( D(x) \frac{\partial u}{\partial x} \right) - V(t) \frac{\partial u}{\partial x} - \lambda u, \quad 0 < x < \ell, \quad t > 0,$$

$$(2.4) \quad -D(0) \frac{\partial u}{\partial x}(t, 0) + V(t)u(t, 0) = G(t)$$

$$(2.5) \quad -D(\ell) \frac{\partial u}{\partial x}(t, \ell) = 0$$

$$(2.6) \quad u(0, x) = \phi(x),$$

where  $\phi$  is the initial distribution of material in the chamber.

The appropriate initial data assumption is closely related to the assumption one makes about the input flux  $G$ . To illustrate possibilities, we can consider several specific situations that arise in geological investigations. A strong argument for steady-state input flux ( $G(t) = \text{constant}$ ) can be made in the case one is investigating a tracer such as lead ( $^{210}\text{Pb}$ ) which exhibits a rather steady production rate from atmospheric (decay of gaseous radon - 222) and oceanic (decay of radon-226) sources. For tracers such as plutonium ( $^{239,240}\text{Pu}$ ) and cesium ( $^{137}\text{Cs}$ ) which result from atmospheric nuclear weapons testing, time dependent flux is more appropriate, and in some cases, for appropriately chosen initial times, the assumption that  $\phi$  vanishes is appropriate. In general though, in both cases one must estimate the initial distribution  $\phi$ , either as a part of the overall inverse problem or, through an a-priori procedure using directly earlier (i.e. deeper)

concentration profiles in the sediment core. Finally, in the case of truly episodic events (ash shards from volcanic eruptions, microtektites of cosmic origin) an impulse input is most appropriate. This can be effectively modeled by choosing an impulse like initial function  $\Phi$  in (2.6) and taking  $G = 0$  in (2.4). The magnitude of this impulse can sometimes be rather easily estimated directly from knowledge of the total material content of the sample.

In any case, to understand the effects of bioturbation on the distribution of material concentrations in core samples, it is sufficient to have values for the parameters  $D$ ,  $V$ ,  $\lambda$ , and  $\ell$ , and, of course, to know that use of these parameter values in the model gives one an accurate quantitative description of concentrations found in core samples. It can be expected that these parameter values will vary depending on the core sample and the material under investigation. Hence one would like to have a procedure whereby given data from a specific core sample, one can, with some confidence, determine the "correct" parameter values. In regard to this inverse procedure, for the model above we note that concentrations in the historical layers (where time in kiloyears can usually be related to centimeters of thickness of core sample e.g., see [11]) represent concentrations at various times at the bottom of the mixing chamber (i.e. at  $x = \ell$ ). Hence data for the process may be given by  $Z(\xi)$  where  $Z(\xi)$  denotes the observed concentration of tracer material at a height of  $\xi$  cm. above the position in the core designated as time  $t = 0$ . In this event a typical inverse problem might be stated: Given observations  $Z(\xi_i)$ ,  $i = 1, 2, \dots, \kappa$  at core locations  $\xi_i$ ,  $i = 1, 2, \dots, \kappa$  find, among some class  $Q$  of admissible parameters, parameters  $q = (D, V, \lambda, \ell)$  that minimize

$$(2.7) \quad J(q) = \sum_{i=1}^{\kappa} |Z(\xi_i) - u(\tau(\xi_i; V), \ell)|^2$$

where  $u$  is the solution to (2.3)-(2.6) corresponding to  $q$  and

$$\tau(\xi; V) = r_V^{-1}(\xi) \quad \text{with} \quad r_V(t) = \int_0^t V(s)ds.$$

In addition to, or in place of some of the parameters in  $q$ , sometimes it is also desirable to estimate  $G$  and/or  $\Phi$  in the formulation above. Of course, in some instances the data from core samples will not support such an inclusive inverse procedure.

The model formulated above is based on the assumption that the entire chamber is available for throughput of material and that the sedimentation rate is the same as the material velocity through the chamber (i.e. no compactification of sediment takes place). In many instances porosity effects and/or compactification are important and should be included in the model. It is also sometimes important to distinguish between tracer materials and sediment particles. These concepts require modifications of the modeling ideas presented above.

We again postulate the moving mixing chamber but (for reasons that will become clear in the sequel) now we let  $z$  denote the chamber coordinates ( $z = 0$  is the water-sediment interface,  $z = l$  is the bottom of the mixing chamber). The porosity  $\phi$  is the fraction of the chamber volume that is available for flow (throughput) so that  $1 - \phi$  is the fraction that is solid. We assume that the porosity  $\phi = \phi(z)$  is depth dependent and let  $\rho_s$  be the constant sediment particle density (in mass per unit length of particulate matter). If we furthermore let  $V = V(t, z)$  be the sediment particle velocity with respect to the  $z$  coordinate system, we may write separate mass balance equations for the sediment particulate matter and tracer. Considering first sediment particles, we have that the particle mass density in the chamber is given by  $\rho_s(1-\phi)$  and the particle mass flux is given by  $j_s = j_s(t, z) = \rho_s(1-\phi)V$ . Assuming conservative particulate matter, we



obtain the sediment mass balance equation

$$(2.8) \quad \frac{\partial}{\partial t} (\rho_s (1-\phi)) + \frac{\partial}{\partial z} (\rho_s (1-\phi)V) = 0.$$

Note that this conservation law implies  $j_s$  is actually independent of  $z$ .

For the tracer, we have similar considerations regarding porosity except the flux is more involved since we have bioturbation and convective movement along with decay. (The sediment particles may also be mixed (ingested, etc) but we cannot measure (observe) this - our observations being of tracer material. Hence the flux for sediment particles only contains a convective movement term.) Let  $c$  denote the mass of tracer per unit mass of sediment particulate matter. Then the tracer mass density (mass per unit length of the chamber) is given by  $c\rho_s(1-\phi)$  and the tracer mass balance equation can be written

$$(2.9) \quad \frac{\partial}{\partial t} (c\rho_s(1-\phi)) + \frac{\partial}{\partial z} (j_T) + \lambda(c\rho_s(1-\phi)) = 0$$

where  $j_T$  is the tracer mass flux. Denoting the tracer velocity by  $V_T$  so that the tracer mass flux is given by  $j_T = c\rho_s(1-\phi)V_T$ , we may divide the tracer mass flux into components representing mixing (bioturbation) and convective flux

$$j_T = c\rho_s(1-\phi)(V_T - V) + c\rho_s(1-\phi)V.$$

The term  $j_M = c\rho_s(V_T - V)$  may be regarded as a "pure" mixing tracer flux (i.e. neglecting porosity) and if we make the Fickian assumption for this flux term

$$j_M = -D \frac{\partial}{\partial z} (c \rho_s),$$

the resulting mixing flux is given by  $-\rho_s(1-\phi) D \frac{\partial c}{\partial z}$ . Hence we have

$$j_T = -\rho_s(1-\phi) D \frac{\partial c}{\partial z} + c \rho_s(1-\phi) V$$

and the tracer mass balance equation (2.9) can be written

$$(2.10) \quad \frac{\partial}{\partial t} (c \rho_s(1-\phi)) + \frac{\partial}{\partial z} (\rho_s(1-\phi) c V) = \frac{\partial}{\partial z} (\rho_s(1-\phi) D \frac{\partial c}{\partial z}) - \lambda \rho_s(1-\phi) c.$$

The sediment mass balance equation (2.8) can be used to modify the tracer equation. Observing that

$$\begin{aligned} \frac{\partial}{\partial t} (c \rho_s(1-\phi)) &= c \frac{\partial}{\partial t} (\rho_s(1-\phi)) + \rho_s(1-\phi) \frac{\partial c}{\partial t} \\ &= -c \frac{\partial}{\partial z} (\rho_s(1-\phi) V) + \rho_s(1-\phi) \frac{\partial c}{\partial t} \\ &= \rho_s(1-\phi) V \frac{\partial c}{\partial z} - \frac{\partial}{\partial z} (c \rho_s(1-\phi) V) + \rho_s(1-\phi) \frac{\partial c}{\partial t} \end{aligned}$$

and using this in (2.10), we obtain

$$(2.11) \quad \rho_s(1-\phi) \frac{\partial c}{\partial t} + \rho_s(1-\phi) V \frac{\partial c}{\partial z} = \frac{\partial}{\partial z} (\rho_s(1-\phi) D \frac{\partial c}{\partial z}) - \lambda \rho_s(1-\phi) c.$$

In the case of constant porosity, this equation reduces to

$$(2.12) \quad \frac{\partial c}{\partial t} + V \frac{\partial c}{\partial z} = \frac{\partial}{\partial z} (D \frac{\partial c}{\partial z}) - \lambda c,$$

which is the same as (2.3) if  $c$  is interpreted as volumetric concentration.

Equation (2.11) can be put in a form similar to (2.3) even when the porosity  $\phi$  is not constant. We define a new independent variable  $x = x(z)$  by

$$x = \int_0^z \rho_s (1-\phi) d\xi.$$

Assuming that  $\rho_s (1-\phi) > 0$ , this defines an invertible mapping between the chamber coordinate variable  $z$  and the new variable  $x$  which is sometimes called the "total sediment particle accumulation". We then have  $\frac{\partial}{\partial z} = \rho_s (1-\phi) \frac{\partial}{\partial x}$  and use of this in (2.11) yields

$$(2.13) \quad \frac{\partial c}{\partial t} + \omega \frac{\partial c}{\partial x} = \frac{\partial}{\partial x} \left( E \frac{\partial c}{\partial x} \right) - \lambda c$$

where  $E \equiv (\rho_s (1-\phi))^2 \mathcal{D}$  and  $\omega \equiv \rho_s (1-\phi) V$  is the particle mass flux (called  $j_s$  above). We see that equation (2.13) has the same form as (2.3) and note that in this equation,  $c$  can be expressed either as tracer mass per unit mass of sediment particulate matter or in the more traditional interpretation as tracer mass per unit length of the sediment column. Also note that in (2.13)  $x$  is no longer simply the vertical distance in the column nor is  $E$  simply the mixing or bioturbation coefficient. Moreover, in such models where porosity and compactification are considered, the concept of "sedimentation rate" is more delicate. To elaborate on this, we may define  $M(t)$ , the total sediment mass at time  $t$  by

$$M(t) = \int_0^{h(t)} \rho_s (1-\phi) d\xi$$

where  $h(t)$  is the sediment column depth measured from some fixed reference coordinate system. Note that  $\frac{dh}{dt}$  represents the rate at which the water-sediment interface is changing relative to a fixed coordinate system and hence is the rate at which the sedimentation layer is increasing. Thus, this is the "true sedimentation rate"  $\bar{V}(t)$  which in general differs from the rate  $V(t,0)$  at which particles are "falling" and passing into the chamber. The porosity is often assumed to have the form

$$\phi(z) = (\phi_0 - \phi_1)e^{-bz} + \phi_1$$

where  $\phi_0 > \phi_1$  if compactification takes place. Moreover, since  $\omega = \frac{dM}{dt}$  is the sediment particle mass flux already defined as  $\rho_s(1-\phi)V$ , we see that

$$\omega(t) = \rho_s(1-\phi(h(t))) \frac{dh}{dt} = \rho_s(1-\phi(z)) V(t,z).$$

Then for  $\phi_0 > \phi_1$  we have

$$\bar{V}(t) = \frac{\omega}{\rho_s(1-\phi(h(t)))} < \frac{\omega}{\rho_s(1-\phi(0))} = V(t,0)$$

or, for a thick sediment column (so that  $\phi \approx \phi_1$ ) we have

$$\bar{V}(t) = \frac{\omega}{\rho_s(1-\phi_1)} < \frac{\omega}{\rho_s(1-\phi_0)} = V(t,0).$$

### 3. THE IDENTIFICATION PROBLEM

In this paper we will concentrate our efforts on the development of numerical approximation schemes for the solution of the parameter estimation problem involving the simplified bioturbation model given by (2.3)-(2.6). Methods applicable to inverse problems for more elaborate models (e.g. those involving porosity and/or compactification effects) are currently under investigation and our findings will be discussed elsewhere.

In this section we give a precise formulation of the identification problem and briefly outline existence, uniqueness and regularity results for solutions to initial-boundary value problems of the form (2.3)-(2.6) which will be required in the subsequent development.

If we make the change of variable  $y = x/\ell$  and allow for the inclusion of a sink/source term  $F = F(t,x)$  in the partial differential equation (2.3) we may, without loss of generality, consider the system for states  $v = v(t,y)$  and parameters  $q = (q_1(y), q_2(t), f(t,y), g(t), \phi(y), \lambda, \ell)$  given by

$$(3.1) \quad \frac{\partial}{\partial t} v(t,y) = \frac{\partial}{\partial y} (q_1(y) \frac{\partial}{\partial y} v(t,y)) - q_2(t) \frac{\partial}{\partial y} v(t,y)$$

$$- \lambda v(t,y) + f(t,y), \quad t > 0, \quad y \in (0,1)$$

$$(3.2) \quad -q_1(0) \frac{\partial}{\partial y} v(t,0) + q_2(t)v(t,0) = g(t), \quad t > 0$$

$$(3.3) \quad -q_1(1) \frac{\partial}{\partial y} v(t,1) = 0, \quad t > 0$$

$$(3.4) \quad v(0,y) = \phi(y), \quad y \in (0,1),$$

where the original states and parameters appearing in (2.3)-(2.6) can be recovered from the relations

$$D(x) = \ell^2 q_1(x/\ell),$$

$$V(t) = \ell q_2(t),$$

$$F(t, x) = f(t, x/\ell),$$

$$G(t) = \ell g(t),$$

$$\Phi(x) = \phi(x/\ell)$$

and

$$u(t, x) = v(t, x/\ell).$$

The least squares performance index (2.7) takes the form

$$(3.5) \quad J(q; v) = \sum_{i=1}^K |Z(\xi_i) - v(\tau(\xi_i; \ell q_2), 1)|^2$$

where  $v$  is the solution to (3.1)-(3.4) corresponding to  $q$ .

In what is to follow we make the standing assumption that the sink/source term  $f$ , the boundary flux  $g$  and initial conditions  $\phi$  are known or have been estimated a-priori. The parameter vector  $q$  is assumed therefore to be of the form  $q = (q_1(y), q_2(t), \lambda, \ell)$ . Treating this somewhat scaled down version of the original identification problem will capture all of the essential features

of our approach and at the same time keep the presentation and discussion as simple as possible. In addition, this formulation is more than adequate to treat the identification problem corresponding to a set of observations involving volcanic ash data which has been the primary focus of our research to date (see [6] and Example 5.3 below). The necessary modifications to our theory so as to allow the estimation of the input terms  $f$  and  $g$  and the initial data  $\phi$  are relatively straightforward and have been discussed in detail elsewhere (see [3], [4]).

We assume  $\phi \in H^0(0,1)$  and that there exists a  $T > 0$ , sufficiently large for which the mappings  $t \mapsto g(t)$  and  $t \mapsto f(t, \cdot)$  are in  $H^0(0,T)$  and  $H^0(0,T;H^0(0,1))$  respectively.

Define

$$Q = C[0,1] \times H^1(0,T) \times R^1 \times R^1$$

with the usual product space topology and let  $Q = Q_1 \times Q_2 \times \Lambda \times L \subset Q$  satisfy the following hypotheses:

- (H1)  $Q_1$  is a compact subset of  $C[0,1]$  and there exist constants  $\mu$  and  $\nu$  such that  $0 < \mu \leq q_1(y) \leq \nu$ ,  $y \in [0,1]$  for all  $q_1 \in Q_1$
- (H2)  $Q_2$  is a compact (with respect to the  $H^1$  topology) subset of  $C^1[0,T]$  with  $0 < \mu \leq q_2(t) \leq \nu$  and  $|\dot{q}_2(t)| \leq \nu$  for all  $t \in [0,T]$  and all  $q_2 \in Q_2$ ,
- (H3)  $\Lambda$  is a compact subset of  $R^1$  with  $0 < \lambda \leq \nu$  for all  $\lambda \in \Lambda$ ,

(H4)  $L$  is a compact subset of  $R^1$  with  $0 < \mu \leq \ell \leq \nu$  for all  $\ell \in L$ .

It is clear that (H1) - (H4) above imply that  $Q$  is a compact subset of  $\mathcal{Q}$ .

Letting  $H = H^0(0,1)$  and  $V = H^1(0,1)$  endowed with the standard Sobolev inner products we have the usual dense embedding  $V \subset H \subset V'$ . For each  $t \in [0,T]$  and  $q = (q_1, q_2, \lambda, L) \in \mathcal{Q}$  define the bilinear form  $L(t; q): V \times V \rightarrow R$  by

$$\begin{aligned} L(t; q)(\chi, \psi) &= \langle q_1 D\chi, D\psi \rangle_0 - q_2(t) \langle \chi, D\psi \rangle_0 \\ &+ \lambda \langle \chi, \psi \rangle_0 + q_2(t) \chi(1) \psi(1), \quad \chi, \psi \in V \end{aligned}$$

and consider the weak form of (3.1)-(3.4) given by

$$(3.6) \quad \langle \dot{v}(t), \psi \rangle_0 + L(t; q)(v(t), \psi) = \langle f(t), \psi \rangle_0 + g(t) \psi(0), \quad t > 0, \psi \in V$$

$$(3.7) \quad v(0) = \phi$$

where  $v(t) = v(t, \cdot)$  and  $f(t) = f(t, \cdot)$ .

Hypotheses (H1) - (H4) imply that for each  $t \in [0,T]$ ,  $q \in \mathcal{Q}$  and  $\chi, \psi \in V$

$$|L(t; q)(\chi, \psi)| \leq 4\nu |\chi|_1 |\psi|_1$$

and that  $L(t; q)(\cdot, \cdot)$  is strongly elliptic. It follows therefore (see [10], Theorem 10.3.4, [21] Theorem III. 5.A.) that it is  $V$ -coercive; that is, there exists an  $\alpha \in R$  such that



$$L(t; q)(\psi, \psi) + \alpha |\psi|_0^2 \geq \beta |\psi|_1^2,$$

$\beta > 0$ , for all  $\psi \in V$  and  $t \in [0, T]$ . If we rewrite the terms on the right hand side of (3.6) as

$$\langle f(t), \psi \rangle_0 + g(t)\psi(0) = \langle \hat{f}(t), \psi \rangle_H$$

where  $\hat{f}(t) = f(t, \cdot) + g(t)\delta(\cdot)$  and  $\delta(\cdot)$  denotes the dirac impulse at zero, then  $\hat{f} \in H^0(0, T; V')$  and standard results (see [14], Theorem III.1.2) yield that the system (3.6), (3.7) admits a unique solution  $v \in C([0, T]; H)$  with  $v \in H^0(0, T; V)$  and  $\dot{v} \in H^0(0, T; V')$ .

Under additional regularity hypotheses on  $q_1, q_2, f, g$  and  $\phi$ , smoother solutions to (3.6), (3.7) can be obtained (see below). When these solutions are sufficiently smooth and  $q_1, q_2, f, g$  and  $\phi$  are sufficiently regular, they coincide with either strong (defined in terms of evolution operators, see [23]) or classical (see [10]) solutions to the original initial boundary value problem (3.1)-(3.4). In light of this, we formally define the identification problem as

(P) Find  $q \in Q$  which minimizes  $J(q; v)$  given by (3.5) where  $v$  is the solution to (3.6), (3.7) corresponding to  $q$ .

As is typically the case with Ritz-Galerkin based methods, in order to demonstrate that our approximation schemes converge, additional regularity of solutions to (3.6), (3.7) will be required. We state the following theorem.

**Theorem 3.1.** Suppose  $q_2 \in C^1[0,T]$ . Let  $n$  be a function in  $C^2([0,T] \times [0,1])$  which satisfies

- (i)  $n(0,y) = \phi(y), \quad y \in (0,1)$
- (ii)  $-q_1(0) \frac{\partial}{\partial y} n(t,0) + q_2(t)n(t,0) = g(t), \quad t > 0$
- (iii)  $-q_1(1) \frac{\partial}{\partial y} n(t,1) = 0, \quad t > 0$

and define

$$h(t,y) = f(t,y) + \frac{\partial}{\partial y} \{q_1(y) \frac{\partial}{\partial y} n(t,y)\} - q_2(t) \frac{\partial}{\partial y} n(t,y) - \lambda n(t,y) - \frac{\partial}{\partial t} n(t,y).$$

If  $h \in C^1([0,T] \times [0,1])$  and

$$\frac{\partial^j}{\partial t^j} h(0,y) = 0, \quad y \in (0,1), \quad j = 0,1,$$

then  $v$ , the solution to (3.6), (3.7) is an element in  $H^1(0,T; H^1(0,1))$  and it can be identified with functions in  $H^1((0,T) \times (0,1))$ .

The proof of Theorem 3.1, which has been omitted, can be argued using Theorem 10.6.17 in [10].

The conditions specified in the statement of Theorem 3.1, which of course are only sufficient conditions, are rather restrictive. However, they can be used to derive specific and not unreasonable conditions on the initial and boundary data  $(\phi, g)$  and parameters  $q_1, q_2$  to insure regularity of solutions to (3.6), (3.7). Although the theorem above is not the most general one possible, it suffices, for our purposes here, to simply demonstrate the

existence of  $H^1(0,T;H^1(0,1))$  solutions. It is in fact the case, that while regularity of solutions is necessary to demonstrate convergence, it has been our experience that it has little or no effect on the actual performance of the schemes when they are applied in practice.

#### 4. APPROXIMATION

In this section we develop approximation schemes to solve the parameter estimation problem (P). Fundamental to our approach is the construction of a sequence of finite dimensional identification problems, each of which has a solution that can be found using conventional techniques and readily available software. We demonstrate that under appropriate hypotheses, solutions to the finite dimensional problems, in some sense, approximate solutions to the original infinite dimensional identification problem (P).

A two stage approximation process is employed. We first use a Ritz-Galerkin approach to approximate the infinite dimensional state equation (3.6) by a sequence of finite dimensional ordinary differential equations. The set of admissible parameters  $Q$ , a subset of the infinite dimensional function space  $Q$  is then discretized. The result is a sequence of optimization problems involving the minimization of a least squares performance index over a compact subset of Euclidean space subject to finite dimensional constraints.

For each  $N = 1, 2, \dots$  let  $V^N$  be a finite dimensional subspace of  $H$  satisfying  $V^N \subset V$ . Suppose  $V^N = \text{span} \{\phi_i^N\}_{i=1}^k$  and define  $P^N: H \rightarrow V^N$  to be the orthogonal projection of  $H$  onto  $V^N$  with respect to the  $H$  (i.e.,  $\langle \cdot, \cdot \rangle_0$ ) inner product. We make the following hypothesis about the approximating properties of the subspaces  $V^N$ .

(H5) For each  $\psi \in H^1(0,1)$ ,  $\|\psi - P^N \psi\|_1 \rightarrow 0$  as  $N \rightarrow \infty$  with  $\|\psi - P^N \psi\|_1 \leq k \|\psi\|_1$  for some constant  $k$  independent of  $N$  and  $\psi$ .

The usual spaces of linear or cubic B-spline functions, among others, are known to satisfy Hypothesis (H5) (see [20], [22]).

The Galerkin equations in  $V^N$  corresponding to the system (3.6), (3.7) are given by

$$(4.1) \quad \langle \dot{v}^N(t), \psi^N \rangle_0 + L(t; q)(v^N(t), \psi^N) = \langle f(t), \psi^N \rangle_0 + g(t)\psi^N(0), \quad t > 0, \quad \psi^N \in V^N$$

$$(4.2) \quad v^N(0) = P^N \phi$$

where  $v^N(t) \in V^N$ ,  $t > 0$ .

The state approximation given by (4.1), (4.2) is the first stage of our approach. We argue that sufficiently smooth solutions to (3.6), (3.7) are approximated by solutions to (4.1), (4.2) with a certain degree of uniformity in  $q$ . The standard arguments (see [3]) yield the convergence of  $v^N(t)$  to  $v(t)$  in the  $H^0$  norm for each  $t \in [0, T]$ . However, since the least squares performance index (3.5) of particular interest to us here involves observations which are pointwise in the spatial variable, we will require that state approximations converge in the stronger  $H^1$  norm.

**Theorem 4.1** Suppose  $\{q^N\}_{N=1}^\infty$  is a sequence in  $Q$  with  $q^N \rightarrow q \in Q$  as  $N \rightarrow \infty$ . Let  $v^N$  denote the solution to (4.1), (4.2) corresponding to  $q^N$  and  $v$  the solution to (3.6), (3.7) corresponding to  $q$ . Then if Hypotheses (H1) - (H5) hold,  $\phi \in H^1(0, 1)$  and  $v \in H^1(0, T; H^1(0, 1))$  we have

$$\lim_{N \rightarrow \infty} \|v^N(t) - v(t)\|_1 = 0$$

for each  $t \in [0, T]$ .

**Proof.**

Let  $q^N = (q_1^N, q_2^N, \lambda^N, \ell^N)$  and  $q = (q_1, q_2, \lambda, \ell)$ .

Now

$$|v^N(t) - v(t)|_1 \leq |v^N(t) - P^N v(t)|_1 + |(P^N - I) v(t)|_1.$$

The regularity assumptions on  $v$  and Hypothesis (H5) imply that the second term on the right hand side of the above estimate tends to zero as  $N \rightarrow \infty$  for each  $t \in [0, T]$ . We therefore need only to consider the term  $|v^N(t) - P^N v(t)|_1$ .

Letting  $z^N(t) = v^N(t) - P^N v(t)$ , (3.6), (3.7) and (4.1), (4.2) yield

$$(4.3) \quad \begin{aligned} \langle \dot{z}^N(t), \psi^N \rangle_0 + L(t; q^N)(z^N(t), \psi^N) &= \langle (I - P^N) \dot{v}(t), \psi^N \rangle_0 + L(t; q)(v(t), \psi^N) \\ &\quad - L(t; q^N)(P^N v(t), \psi^N), \end{aligned} \quad t > 0, \psi^N \in V^N$$

$$(4.4) \quad z^N(0) = 0.$$

In order to simplify the presentation, we suppress the display of explicit  $t$  dependence. Choosing  $\psi^N = \dot{z}^N$ , we rewrite (4.3) as

$$\begin{aligned} &|\dot{z}^N|_0^2 + \frac{1}{2} \frac{d}{dt} |\sqrt{q_1^N} Dz^N|_0^2 + \frac{1}{2} \frac{d}{dt} \{q_2^N [z^N]_1^2\} - \\ &\frac{1}{2} q_2^N [z^N]_1^2 + \frac{1}{2} \frac{d}{dt} |\sqrt{\lambda^N} z^N|_0^2 - \frac{d}{dt} \{q_2^N \langle z^N, Dz^N \rangle_0\} \\ &+ q_2^N \langle z^N, Dz^N \rangle_0 + q_2^N \langle \dot{z}^N, Dz^N \rangle_0 \\ &= \langle (I - P^N) \dot{v}, \dot{z}^N \rangle_0 + \frac{d}{dt} \langle \Delta_1^N, Dz^N \rangle_0 \end{aligned}$$

$$- \langle \dot{\Delta}_1^N, Dz^N \rangle_0 + \frac{d}{dt} \langle \Delta_2^N, Dz^N \rangle_0 - \langle \dot{\Delta}_2^N, Dz^N \rangle_0$$

$$+ \langle \Delta_\lambda^N, \dot{z}^N \rangle_0 - \frac{d}{dt} \{ [\Delta_2^N]_1 [z^N]_1 \} + [\dot{\Delta}_2^N]_1 [z^N]_1$$

where  $\Delta_1^N(t) = q_1 Dv(t) - q_1^N D P^N v(t)$ ,  $\Delta_2^N(t) = q_2^N(t) P^N v(t) - q_2(t) v(t)$ ,

$\Delta_\lambda^N(t) = \lambda v(t) - \lambda^N P^N v(t)$  and  $[w]_1 = [w(t, \cdot)]_1 = w(t, 1)$ .

Hypothesis (H2) together with repeated application of the inequality

$$(4.5) \quad \langle \chi, \psi \rangle \leq c |\chi|^2 + \frac{1}{4c} |\psi|^2, \quad c > 0$$

yield

$$|\dot{z}^N|_0^2 + \frac{1}{2} \frac{d}{dt} \{ |\sqrt{q_1^N} Dz^N|_0^2 + q_2^N [z^N]_1^2 + \lambda^N |z^N|_0^2 \}$$

$$\leq \frac{\nu}{2} |z^N|_1^2 + \nu \left\{ \frac{1}{2} |z^N|_0^2 + \frac{1}{2} |Dz^N|_0^2 \right\} +$$

$$\nu \left\{ c_1 |\dot{z}^N|_0^2 + \frac{1}{4c_1} |Dz^N|_0^2 \right\} + \frac{d}{dt} \{ q_2^N \langle z^N, Dz^N \rangle_0 +$$

$$\langle \Delta_1^N, Dz^N \rangle_0 + \langle \Delta_2^N, Dz^N \rangle_0 - [\Delta_2^N]_1 [z^N]_1 \} +$$

$$+ \frac{1}{4c_1} |(I - P^N) \dot{v}|_0^2 + c_1 |\dot{z}^N|_0^2 + \frac{1}{2} |\dot{\Delta}_1^N|_0^2 + \frac{1}{2} |Dz^N|_0^2$$

$$+ \frac{1}{2} |\dot{\Delta}_2^N|_0^2 + \frac{1}{2} |Dz^N|_0^2 + \frac{1}{4c_1} |\Delta_\lambda^N|_0^2 + c_1 |\dot{z}^N|_0^2 + \frac{1}{2} [\dot{\Delta}_2^N]_1^2 + \frac{1}{2} [z^N]_1^2.$$

Choosing  $c_1$  such that  $(\nu+2)c_1 < 1$ , we can eliminate terms involving  $|\dot{z}^N|_0^2$

from the above expression to obtain

$$\begin{aligned}
 (4.6) \quad & \frac{1}{2} \frac{d}{dt} \{ |q_1^N \bar{Dz}^N|_0^2 + q_2^N |z^N|_1^2 + \lambda^N |z^N|_0^2 \} \\
 & < \frac{\nu+1}{2} |z^N|_1^2 + \frac{\nu}{2} |z^N|_0^2 + \left( \frac{\nu}{2} + \frac{\nu}{4c_1} + 1 \right) |Dz^N|_0^2 \\
 & + \frac{1}{4c_1} |(I - P^N) \dot{v}|_0^2 + \frac{1}{2} |\dot{\Delta}_1^N|_0^2 + \frac{1}{2} |\dot{\Delta}_2^N|_0^2 \\
 & + \frac{1}{4c_1} |\Delta_\lambda^N|_0^2 + \frac{1}{2} |\dot{\Delta}_2^N|_1^2 + \frac{d}{dt} \{ q_2^N \langle z^N, Dz^N \rangle_0 \\
 & + \langle \Delta_1^N, Dz^N \rangle_0 + \langle \Delta_2^N, Dz^N \rangle_0 - |\Delta_2^N|_1 |z^N|_1 \}.
 \end{aligned}$$

Integrating (4.6) from 0 to  $t$ , applying Hypothesis (H1) - (H3) and recalling (4.4) we find

$$\theta^N(t) \leq K \int_0^t \theta^N(s) ds + \int_0^t \rho^N(s) ds + \sigma^N(t) - \sigma^N(0)$$

where

$$\theta^N(t) = |z^N(t)|_1^2 + |z^N(t)|_0^2 + |Dz^N(t)|_0^2,$$

$$\rho^N(t) = \frac{1}{4c_1} |(I - P^N) \dot{v}(t)|_0^2 + \frac{1}{2} |\dot{\Delta}_1^N(t)|_0^2 + \frac{1}{2} |\dot{\Delta}_2^N(t)|_0^2$$

$$+ \frac{1}{4c_1} |\Delta_\lambda^N(t)|_0^2 + \frac{1}{2} |\dot{\Delta}_2^N(t)|_1^2,$$

$$\sigma^N(t) = q_2^N(t) \langle z^N(t), Dz^N(t) \rangle_0 + \langle \Delta_1^N(t), Dz^N(t) \rangle_0$$

$$+ \langle \Delta_2^N(t), Dz^N(t) \rangle_0 - |\Delta_2^N(t)|_1 |z^N(t)|_1$$

$$\text{and } K = \frac{\nu+2}{\mu} + \frac{\nu}{2\mu c_1}.$$



Once again employing (4.5) we obtain

$$\begin{aligned} \sigma^N &\leq \nu \left\{ \frac{1}{4c_2} |z^N|_0^2 + c_2 |Dz^N|_0^2 \right\} + \frac{1}{4c_2} |\Delta_1^N|_0^2 \\ &+ c_2 |Dz^N|_0^2 + \frac{1}{4c_2} |\Delta_2^N|_0^2 + c_2 |Dz^N|_0^2 \\ &+ \frac{1}{4c_2} |\Delta_2^N|_1^2 + c_2 |z^N|_1^2 \\ &\leq \frac{\nu}{4c_2} |z^N|_0^2 + c_3 \theta^N + \Delta^N \end{aligned}$$

where  $c_3 = (\nu+2)c_2$  and

$$\Delta^N(t) = \frac{1}{4c_2} \{ |\Delta_1^N(t)|_0^2 + |\Delta_2^N(t)|_0^2 + |\Delta_2^N(t)|_1^2 \}.$$

Choosing  $c_2$  such that  $c_3 < 1$ , we obtain

$$(4.7) \quad \theta^N(t) \leq \beta^N(t) + \frac{K}{1-c_3} \int_0^t \theta^N(s) ds$$

where

$$\beta^N(t) = \frac{1}{1-c_3} \left\{ \int_0^T \rho^N(s) ds + \Delta^N(0) + \Delta^N(t) + \frac{\nu}{4c_2} |z^N(t)|_0^2 \right\}.$$

Applying the Gronwall inequality to (4.7), the desired result will follow once we have shown that  $\beta^N(t) \rightarrow 0$  as  $N \rightarrow \infty$  for each  $t \in [0, T]$ . The assumption that  $\nu \in H^1(0, T; H^1(0, 1))$  together with standard estimates yield

$$\begin{aligned} (4.8) \quad \int_0^T \rho^N(s) ds &\leq K_1 \{ |q_1^N - q_1|_\infty^2 + |q_2^N - q_2|_1^2 + |\lambda^N - \lambda|^2 \} \|\nu\|_1^2 \\ &+ K_2 \|(I - P^N)\nu\|_1^2, \end{aligned}$$

$$(4.9) \quad \Delta^N(t) \leq K_3 \{ |q_1^N - q_1|_\infty^2 + |q_2^N - q_2|_\infty^2 \} |v(t)|_1^2 + K_4 |(I - P^N) v(t)|_1^2$$

and

$$(4.10) \quad \Delta^N(0) \leq K_3 \{ |q_1^N - q_1|_\infty^2 + |q_2^N - q_2|_\infty^2 \} |\phi|_1^2 + K_4 |(I - P^N)\phi|_1^2$$

where  $K_i$ ,  $i = 1, 2, 3, 4$  is a constant which does not depend on  $N$  or  $q \in Q$ .

It is immediately clear from (4.8), (4.9) and (4.10) that Hypothesis (H5) together with the assumptions that  $v \in H^1(0, T; H^1(0, 1))$  and  $\phi \in H^1(0, 1)$  imply  $\int_0^T \rho^N(s) ds \rightarrow 0$ ,  $\Delta^N(0) \rightarrow 0$  and  $\Delta^N(t) \rightarrow 0$  for each  $t \in [0, T]$  as  $N \rightarrow \infty$ . Arguments similar in spirit to those above, although greatly simplified, can be used to show (see [3])  $|z^N(t)|_0^2 \rightarrow 0$  as  $N \rightarrow \infty$  for each  $t \in [0, T]$ . We conclude therefore that  $\beta^N(t) \rightarrow 0$  as  $N \rightarrow \infty$  for each  $t \in [0, T]$  and the theorem is proven.

An application of the Sobolev embedding theorem (see [21]) yields the following corollary.

**Corollary 4.1.** Under the hypotheses of Theorem 4.1 we have

$$\lim_{N \rightarrow \infty} \{ \sup_{[0, 1]} |v^N(t) - v(t)| \} = 0$$

for each  $t \in [0, T]$ .

We consider next the second stage of approximation; the discretization of the set of admissible parameters,  $Q$ .

For each  $m = 1, 2, \dots$  we consider approximation spaces

$$S_m^1 \subset C[0, 1], S_m^1 = \text{span} \{ \psi_m^i \}_{i=1}^{\mu_m} \quad \text{and} \quad S_m^2 \subset H^1(0, T), S_m^2 = \text{span} \{ \chi_m^i \}_{i=1}^{\nu_m} \quad \text{and let}$$

$I_m, J_m$  denote mappings  $I_m : C[0,1] \rightarrow S_m^1$ ,  $J_m : H^1(0,T) \rightarrow S_m^2$ . For each  $M = (m_1, m_2)$  with  $m_i \in \mathbb{Z}^+$ ,  $i = 1, 2$  define  $Q_M \subseteq S_{m_1}^1 \times S_{m_2}^2 \times \Lambda \times L \subset Q$  by

$$(4.11) \quad Q_M \equiv I_M(Q) \equiv I_{m_1}(Q_1) \times J_{m_2}(Q_2) \times \Lambda \times L.$$

We shall require the following hypotheses on the mappings  $I_M$ :

(H6) The mapping  $I_M : Q \rightarrow Q$  is continuous

(H7) For each  $q \in Q$ ,  $I_M(q) \rightarrow q$  as  $m_1, m_2 \rightarrow \infty$  with the convergence uniform in  $q \in Q$ .

Note that  $Q$  compact together with Hypothesis (H6) imply that  $Q_M$  is a compact subset of  $Q$ . Note also that we do not require  $Q_M \subset Q$ .

Once again typical choices for  $S_m^1$  and  $S_m^2$  are spaces of linear or cubic spline functions corresponding to meshes  $\Delta = 1/m$  and  $\Delta = T/m$  respectively with the mappings  $I_m$  and  $J_m$  being the usual interpolation operators. Under appropriate assumptions on  $Q$ , it is not difficult to show that these choices lead to discretizations which satisfy hypotheses (H6) and (H7). (See [4], [5]).

We consider the system (4.1), (4.2) for  $q_M \in Q_M$ . We obtain the initial value problem in  $R^{k^N}$  given by

$$(4.12) \quad M^N \dot{w}^N(t) + L_M^N(t; \alpha) w^N(t) = F^N(t)$$

$$(4.13) \quad w^N(0) = (M^N)^{-1} w_0^N$$

where  $\alpha = (\alpha^1, \alpha^2, \alpha^3, \alpha^4) \in \Omega_M$ , a compact subset of  $R^{\mu_{m1}} \times R^{\nu_{m2}} \times R^1 \times R^1$  and

$$(4.14) \quad [M^N]_{ij} = \langle \phi_i^N, \phi_j^N \rangle_0,$$

$$(4.15) \quad [L_M^N(t; \alpha)]_{ij} = \sum_{k=1}^{\mu_{m1}} \alpha_k^1 \langle \psi_{m1}^k D\phi_i^N, D\phi_j^N \rangle_0 \\ - \sum_{k=1}^{\nu_{m2}} \alpha_k^2 \chi_{m2}^k(t) \{ \langle D\phi_i^N, \phi_j^N \rangle_0 - \phi_i^N(1) \phi_j^N(1) \} + \alpha^3 \langle \phi_i^N, \phi_j^N \rangle_0,$$

$$(4.16) \quad F_i^N(t) = \langle f(t), \phi_i^N \rangle_0 + g(t) \phi_i^N(1)$$

$$(4.17) \quad w_{0i}^N = \langle \phi, \phi_i^N \rangle_0$$

$i, j = 1, 2, \dots, k^N$  and

$$v^N(t) = \sum_{i=1}^{k^N} w_i^N(t) \phi_i^N.$$

We define the sequence of approximating identification problems as:

( $P_M^N$ ) Find  $q_M^* \in Q_M$  which minimizes over  $Q_M$  the functional  $J(q; v^N)$  given by (3.5) where  $v^N$  is the solution to (4.1), (4.2) corresponding to  $q$ ,

or equivalently:

Find  $\alpha^* \in \Omega_M$  which minimizes

$$J_M^N(\alpha; w^N) = \sum_{i=1}^{\kappa} |Z(\xi_i) - \sum_{j=1}^{k^N} w_j^N(\tau(\xi_i; \alpha^4 \sum_{k=1}^{\nu_{m2}} \alpha_k^2 \chi_{m2}^k)) \phi_j^N(1)|^2$$

where  $w^N$  is the solution to (4.12), (4.13) corresponding to  $\alpha$ .

It is immediately clear that for each  $N, M$  and  $\alpha \in \Omega_M$  the system (4.12), (4.13) admits a unique solution which depends continuously upon  $\alpha$ . We have therefore, that for each  $N$  and  $M$ , problem  $(P_M^N)$  has a solution  $(q_M^N)^* \in Q_M$ . Since  $Q_M = I_M(Q)$ , there exists  $\bar{q}_M^N \in Q$  such that

$I_M(\bar{q}_M^N) = (q_M^N)^*$ . Now  $Q$  is compact. Therefore, there exist  $\{\bar{q}_{M_k}^{N_j}\} \subset \{\bar{q}_M^N\}$  and an element  $q^* \in Q$  such that  $\bar{q}_{M_k}^{N_j} \rightarrow q^*$  in  $Q$  as  $j, k \rightarrow \infty$ . This subsequence can always be chosen so that  $N_j \rightarrow \infty$  and  $(m_1)_k, (m_2)_k \rightarrow \infty$  as  $j, k \rightarrow \infty$ . Now

$$J((q_{M_k}^{N_j})^*; v^{N_j}) \leq J(q; v^{N_j}), \quad q \in Q_{M_k}$$

and consequently, from (4.11), we have

$$(4.18) \quad J((q_{M_k}^{N_j})^*; v^{N_j}) \leq J(I_{M_k}(q); v^{N_j}), \quad q \in Q.$$

Hypothesis (H7) and

$$\|(q_{M_k}^{N_j})^* - q^*\|_Q \leq \|I_{M_k}(\bar{q}_{M_k}^{N_j}) - \bar{q}_{M_k}^{N_j}\|_Q + \|\bar{q}_{M_k}^{N_j} - q^*\|_Q$$

imply  $(q_{M_k}^{N_j})^* \rightarrow q^*$  in  $Q$  as  $j, k \rightarrow \infty$ . Taking the limit as  $j, k \rightarrow \infty$  in (4.18)

and applying Corollary 4.1 (with an appropriate re-indexing and the assumption that the necessary regularity conditions are satisfied) we obtain

$$J(q^*; v^*) \leq J(q; v), \quad q \in Q$$

where  $v^*$  denotes the solution to (3.6), (3.7) corresponding to  $q^*$ ; or that  $q^*$  is a solution to problem (P).

We summarize these results in the following theorem.

**Theorem 4.2** For each  $N = 1, 2, \dots$  and  $M \in \mathbb{Z}^+ \times \mathbb{Z}^+$  let problem  $(P_M^N)$  be as it has been defined above. Then if hypotheses (H1) - (H7) hold, each problem  $(P_M^N)$  has a solution  $(q_M^N)^*$ . The sequence  $\{(q_M^N)^*\}$  admits a  $Q$ -convergent subsequence, the limit of which,  $q^*$ , is an element of  $Q$ . If  $\phi \in H^1(0,1)$  and  $v^*$ , the solution to (3.6), (3.7) corresponding to  $q^*$  is an element in  $H^1(0,T; H^1(0,1))$  then  $q^*$  is a solution to problem (P). Moreover, for any convergent subsequence  $\{(\bar{q}_{M_k}^N)^*\} \subset \{(q_M^N)^*\}$  with  $(\bar{q}_{M_k}^N)^* \rightarrow q^*$ ,  $N_1 \rightarrow \infty$  and  $(m_1)_k$ ,  $(m_2)_k \rightarrow \infty$  as  $j, k \rightarrow \infty$  and  $\bar{v}^* \in H^1(0,T; H^1(0,1))$  we have that  $\bar{q}^*$  is a solution to problem (P).

## 5. Numerical Results

In this section we present a brief summary of some preliminary numerical results. Our primary intent here is to simply demonstrate the feasibility and efficacy of our approach. A more complete study involving a somewhat broader spectrum of examples (including pathologies) and more sophisticated approaches to solving the approximating optimization problems will be discussed in detail elsewhere.

We consider inverse problems for systems of the form (2.3)-(2.6) involving the estimation of a spatially varying diffusivity coefficient  $\mathcal{D} = \mathcal{D}(x)$ . We assume that the advection rate  $V$  is constant in time, that there is no boundary flux and that all parameters, with the exception of the diffusivity, are known. We also allow for the inclusion of a sink/source term,  $F = F(t, x)$  in (2.3).

Transforming both the space and time coordinates to dimensionless variables;  $y = x/\ell$ ,  $s = Vt/\ell$ , we obtain

$$(5.1) \quad \frac{\partial}{\partial s} v(s, y) = \frac{\partial}{\partial y} \{q(y) \frac{\partial}{\partial y} v(s, y)\} - \frac{\partial}{\partial y} v(s, y) - \alpha v(s, y) + f(s, y), \quad s > 0, \quad y \in (0, 1)$$

$$(5.2) \quad -q(0) \frac{\partial}{\partial y} v(s, 0) + v(s, 0) = 0 \quad s > 0$$

$$(5.3) \quad -q(1) \frac{\partial}{\partial y} v(s, 1) = 0 \quad s > 0$$

$$(5.4) \quad v(0, y) = \phi(y) \quad y \in (0, 1)$$

where  $v(s, y) = u(\ell s/V, \ell y)$ ,  $q(y) = \mathcal{D}(\ell y)/\ell V$ ,  $\alpha = \ell \lambda/V$ ,  $f(s, y) = \ell F(\ell s/V, \ell y)/V$ ,

and  $\phi(y) = \phi(\ell y)$ .

In addition, for our discussions here, we assume that observations  $\{\varepsilon_{ij}\}_{i=1,\dots,\mu}$  for  $v$  (equivalently,  $u$ ) at times  $s_i$ ,  $i = 1, \dots, \mu$  and positions  $y_j$ ,  $j = 1, \dots, \nu$  have been provided and consider the least squares performance index of the form

$$J(q; v) = \sum_{i=1}^{\mu} \sum_{j=1}^{\nu} |v(s_i, y_j) - \varepsilon_{ij}|^2$$

where  $v$  is the solution to (5.1) - (5.4) corresponding to  $q$ .

All computations were performed on IBM 3081 processors at Brown University and the University of Southern California. The approximating state spaces  $V^N$  were chosen as the span of cubic B-splines defined with respect to the uniform partition  $\{0, 1/N, 2/N, \dots, 1\}$  of the interval  $[0, 1]$ . The set of admissible parameters was discretized using linear spline functions with respect to the mesh  $\{0, 1/M, 2/M, \dots, 1\}$ . Note that in this case we have  $k^N = N + 3$  and  $\mu_M = M + 1$ . The inner products in (4.14) - (4.17) were computed using a composite two point Gauss-Legendre quadrature formula. The use of B-spline bases leads to banded generalized mass  $(M^N)$  and stiffness  $(L_M^N)$  matrices.

The finite dimensional optimization problems  $(P_M^N)$  were solved using an iterative Levenberg-Marquardt scheme as implemented in the IMSL Library routine ZXSSQ. Gradients and Jacobians are computed by the routine using finite difference approximation with rank one updates in each iteration. We also attempted to solve the finite dimensional optimization problems using a quasi-Newton algorithm, a scheme due to Broyden, Fletcher, Goldfarb and Shanno (BFGS) (see [9]), with analytical gradients computed using a co-state formulation (see [2], [8]). Our preliminary findings point to the conclusion



that the latter approach is inferior. We found that it was extremely difficult to obtain accurate search directions with the gradients computed in this manner. However, we are continuing to investigate these ideas with the intent of improving numerical performance.

In the examples that follow, the compactness constraints on the set of admissible parameters  $Q$  were not explicitly enforced when the finite dimensional optimization problems were solved. As could be expected, this did lead to some conditioning problems when  $M$  became large. The use of a constrained optimization package to solve the finite dimensional optimization problems is currently under study.

The initial value problems (4.12), (4.13) in  $R^{k^N}$  were solved in each iteration using Gear's method (IMSL Library routine DGEAR) for stiff systems.

### EXAMPLE 5.1

We consider the system (5.1) - (5.4) with

$$\begin{aligned} q(y) &= 1 + y^2, \\ f(s, y) &= (2 - 8y + 1y^2)e^{-s}, \\ \phi(y) &= 2 + 2y - y^2 \end{aligned}$$

and  $\alpha = 0$ . We estimated  $q$  from observations at  $\{(s_i, y_j)\}_{i=0,1,2,\dots,8; j=0,1,2,\dots,4}$  generated using the true solution to the system

$$(5.5) \quad v(s, y) = (2 + 2y - y^2)e^{-s}$$

where  $s_i = .25i$  and  $y_j = .25j$ . The initial estimate for  $q$  supplied to the

optimization routine was taken to be

$$q^0(y) = 1, \quad 0 \leq y \leq 1.$$

Our results with  $N = 32$  and various values of  $M$  are summarized in Table 5.1 below. The case  $M = 0$  corresponds to the best fit taking  $q$  to be constant over the entire interval.

$y$	$q_0^*(y)$	$q_1^*(y)$	$q_2^*(y)$	$q_3^*(y)$	$q_4^*(y)$	$q(y)$
0.0	1.172	0.920	0.961	0.978	0.987	1.000
0.1	1.172	0.992	1.006	1.014	1.015	1.010
0.2	1.172	1.065	1.052	1.050	1.042	1.040
0.3	1.172	1.137	1.097	1.085	1.092	1.090
0.4	1.172	1.209	1.143	1.164	1.164	1.160
0.5	1.172	1.282	1.208	1.264	1.236	1.250
0.6	1.172	1.354	1.354	1.364	1.363	1.360
0.7	1.172	1.426	1.500	1.479	1.490	1.490
0.8	1.172	1.498	1.645	1.624	1.637	1.640
0.9	1.172	1.571	1.791	1.769	1.804	1.810
1.0	1.172	1.643	1.937	1.914	1.972	2.000
$J(q_M^*)$	$6. \times 10^{-3}$	$2. \times 10^{-4}$	$4. \times 10^{-6}$	$3. \times 10^{-6}$	$3. \times 10^{-6}$	
CPU (M:S)	0:49.92	1:00.53	1:29.49	2:02.02	2:35.82	

TABLE 5.1

### EXAMPLE 5.2

In this example we estimate the non-monotone, single peak function  $q$  given by

$$q(y) = (1 + ay)e^{-by}$$

with  $a = 10.43$  and  $b = 2.43$ . Taking  $\alpha = 0$ ,

$$f(s,y) = (y^2(e^{by} - 2ab) + y(2ab + 4a - 2b) + (2b - 2a + 2 - 4e^{by}))e^{-(s+by)},$$

and

$$\phi(y) = 2 + 2y - y^2.$$

The true solution to the system is again given by (5.5). Using the same observation points as in the previous example, setting

$$q^0(y) = 1.5, \quad 0 < y < 1$$

and taking  $N = 6$  and  $M = 4$ , we obtained the fit for  $q$  shown in Figure 5.1 below.

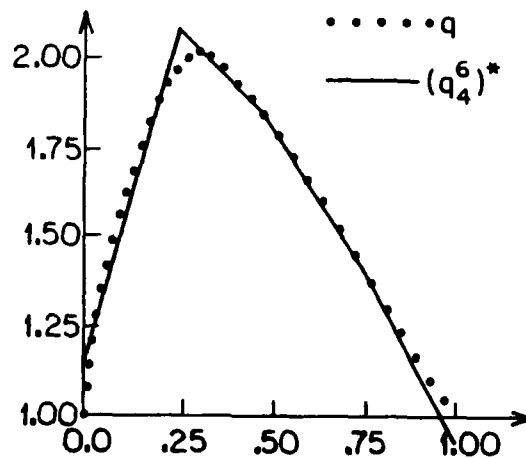


FIGURE 5.1

The residual was  $J((q_4^6)^*) = 3. \times 10^{-6}$ .

The scheme performed well when  $N$  and  $M$  were chosen relatively small. Increasing either  $N$  or  $M$  independently yielded some improvement initially. However, this was followed by the onset of ill conditioning in the finite dimensional optimization problems as the number of degrees of freedom in either the state or the parameter space discretizations were increased. (Based on our initial computational findings with other examples, we anticipate that enforcing the compactness constraints on the set of admissible parameters will remedy this situation.) The scheme also began to have some difficulty if the parameters  $a$  and  $b$  were chosen so as to cause the total variation of  $q$  to be too large.

### EXAMPLE 5.3

We estimate a depth dependent bioturbation coefficient using a set of observations from a volcanic ash concentration profile measured in a sediment core sample taken in the North Atlantic. We consider the model given by (5.1) - (5.4) with  $\alpha = 0$  (we are dealing with a non-radioactive or conservative tracer),  $f = 0$  and

$$(5.6) \quad \phi(y) = m\delta(y)$$

where  $\delta$  denotes the unit impulse at zero and  $m$  is the total mass of ash in the sample as determined from the data.

We were provided with the estimate  $V = 2.5$  cm/kyr for the sedimentation rate in the region where the core sample from which our ash data came was taken. In addition, by invoking (possibly inappropriately in the presence of depth dependent mixing) the observation in [11] that the concentration-

weighted mean depth of the ash profile in the historical layers is the depth in the core at which the ash layer would have been observed had no mixing taken place, we estimate  $\ell$ , the depth to which mixing takes place (see [6]) to be 17.25 cm.

Using the estimates for  $V$  and  $\ell$  given above we are able to convert the depth scale on which our data is specified to an equivalent  $s$ -scale. Our observations turn out to be given at temporal locations  $s_i = .144925i$ ,  $i = 0, 1, 2, \dots, 16$  and of course all at the spatial location  $y = 1$ .

We set  $N = 32$  and used our scheme to estimate  $q$  for various values of  $M$ . We approximated the impulse initial conditions (5.6) by

$$\phi(y) \approx m\hat{\phi}_2^{32}(y)$$

where  $\hat{\phi}_2^{32}$  denotes the normalized ( $\int_0^1 \hat{\phi}_2^{32} = 1$ ) cubic B-spline corresponding to the uniform mesh  $\{0, 1/32, 2/32, \dots, 1\}$  which is centered over zero. This approximation is justified by the relatively narrow support of the B-splines and the fact that it eliminates the error which would be introduced if any other impulse function approximation were projected onto the subspace of splines.

The initial estimate for  $q$  was taken to be

$$q^0(y) = .02198, \quad 0 < y < 1,$$

the optimal estimate for  $q$  obtained in [6] using this set of observations and the assumption that the mixing intensity is constant throughout the mixed layer.

The model (5.1) - (5.4) with depth dependent mixing rate yielded some, although not a significant, reduction in the residual when compared to the fit obtained using a constant mixing rate model. (See Figure 5.2 below.)

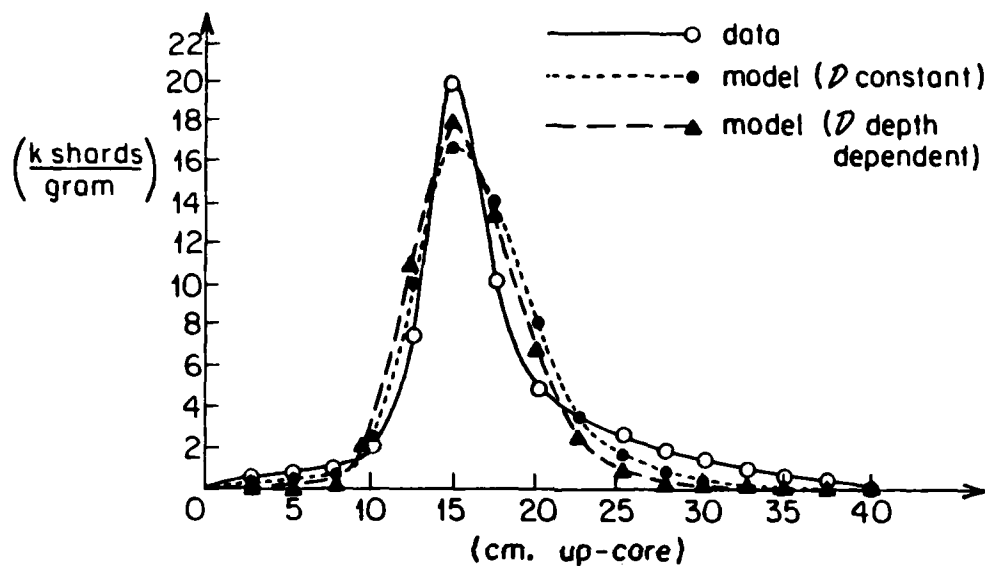


FIGURE 5.2

In addition the optimal mixing rate profiles produced by our scheme did not agree with the widely accepted hypothesis that mixing is most intense near the sea floor/sea interface and then decreases with depth (see Figure 5.3).

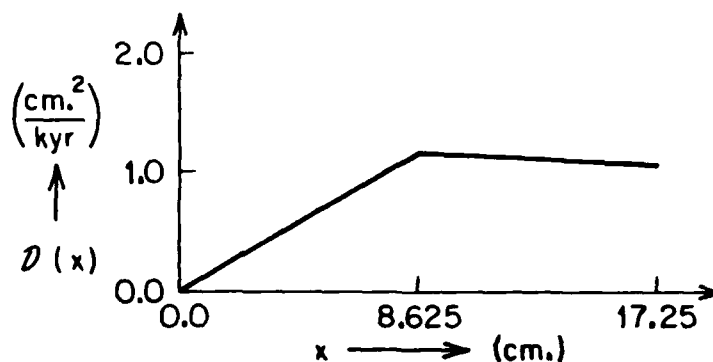


FIGURE 5.3

Based upon these findings, we conclude therefore that the inclusion of a depth dependent mixing rate alone can not significantly improve our ability to explain this set of observations. Other enhancements of the original model, (e.g., time dependent sedimentation rate, porosity and/or compactification effects) must be considered. The scheme developed here should prove to be a valuable tool in the investigation and evaluation of these modeling ideas.

**ACKNOWLEDGEMENT** The authors would like to gratefully acknowledge Mr. Chunming Wang for the assistance he provided in carrying out the computations discussed in this paper and Professors John Imbrie and Warren Prell of the Department of Geological Sciences of Brown University for their continued encouragement and stimulating remarks on this work. They would also like to thank them for supplying the volcanic ash data from the laboratory of Dr. William Ruddiman of The Lamont-Doherty Geological Observatory of Columbia University which was used in Example 5.3.

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